NTNU **Institutt for fysikk**

Contact during the exam:
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Exam in TFY4235/FY8904 Computational Physics

May 04, 2020
09:00

Allowed help: Alternativ **A**

This problem set consists of 8 pages.

This exam is published on Monday, May 04 at 09:00 hours. You can work on your solution till **Fri. May 08, 2020 at 23:00** ("the deadline"). Before the deadline you should submit your final report in the pdf-format and a zip-file containing the documented source code. For the names of the files that you will submit, please use `<lastname>_TFY4235_report.pdf` and `<lastname>_TFY4235_code.zip`; for those of you taking the course using the FY8904 code, replace TFY4235 with by this code. The submission of your work you will do via the system "Inspera" that you can find at `https://ntnu.inspera.no/`. You will receive an email at the start of the exam, detailing how to log in to this system and how to submit your report via it.

Prior to the deadline you are *also* expected[1], to send the final report to me at email `Ingve.Simonsen@ntnu.no` with subject TFY4235 or FY8904.[2]

[1] Useful in the unlikely event that something should go wrong with the digital submission via "Inspera" (or you cannot get it to work properly).

[2] Warning: If your email is too large, the gmail system, to which I also forward my email, may notify you that the message was too large to be delivered to my gmail account. This means that your message was received successfully by the ntnu email system, if you were not informed otherwise.

There are no constraints on the kind of aid you may want to use in connection with this exam, including discussing it with anybody. However, *the report and the computer code you will have to write yourself*. Please attach your computer codes as appendices to the report. Give as a footnote the names of your collaborators during the exam. The report may be written in either Norwegian (either variants) or in English.

Should you run out of time, you are adviced to spend the time on properly explaning what you did and the results you obtained instead of following a strategy of doing a little bit here-and-there without much explanation.

Information posted during the exam, like potential misprints, links to papers, extended deadline etc. will be posted on the web-page of the course at `http://web.phys.ntnu.no/~ingves/Teaching/TFY4235/Exam/`. It is your responsibility to *check this information regularly!*

There are no formal requirements for the format of the report in addition to what was said above. The report should explain what you have been doing, your results, and how you interpret these results. Details should be included to the extent that we as graders can follow your way of reasoning. General background theory that, for instance, can be found in textbooks, is not needed in the report. It is documentation of your work we are interested in! Remember that if you have written an original and/or clever code for solving the problem, but are not able to explain it well in the report, it is hard to give you full credit.

The first point of contact for questions to this exam are the TAs

- Guillermo Garrido Hernandez (guillermo.g.hernandez@ntnu.no)
- Mohammad Alidoust (mohammad.alidoust@ntnu.no)

Good luck to everyone of you!

Problem 1

Your suggested solution for *Assignment no 2* [1] should be handed in as part of the report. It will count 15% towards the final grade of the course.

Problem 2

This exam problem is related to the study of a certain property of the two-dimensional Ising model on a square lattice [2]. Lars Onsager, a graduate from NTNU in the 1920s and the 1968 Nobel laureate in chemistry, solved this model analytically [3]. In particular, he demonstrated that it displays a phase transition for a critical temperature.

2.1 Ising model

The Ising model is a model of interacting spins placed on a lattice. When this model is implemented on a square lattice the Hamiltonian (energy function) has the form

$$H = -\frac{J}{2} \sum_{\langle \mathbf{m},\mathbf{n} \rangle} \sigma_{\mathbf{m}} \sigma_{\mathbf{n}}, \tag{1}$$

where $\sigma_{\mathbf{m}} = \pm 1$ is the spin at node $\mathbf{m}$ of the lattice and the sum over $\langle \mathbf{m}, \mathbf{n} \rangle$ runs over all nearest neighbors; spins with $\sigma_{\mathbf{m}} = 1$ and $\sigma_{\mathbf{m}} = -1$ are traditionally referred to as *spin up* and *spin down*, respectively. Hence, for each node $\mathbf{m}$, we sum over its four nearest neighbors $\mathbf{n}$. This leads to double counting, explaining the prefactor $1/2$ that appears on the right-hand side of Eq. (1). The coupling strength J is a positive constant and in the following, for simplicity, we will assume $J = 1$.

We now describe the square lattice. We orient it with respect to a cartesian coordinate system (x, y) so that the principal axes coincide with the axes of the coordinate system. Hence, the node address $\mathbf{m}$ can be written $\mathbf{m} = (i_m, j_m)$, where (the integer) i_m is the coordinate of $\mathbf{m}$ along the x axis and j_m is the coordinate of $\mathbf{m}$ along the y axis. We limit the size of the lattice to the two intervals $1 \leq i_m \leq N_x$ and $1 \leq j_m \leq N_y$.

2.2 Line tension

2.2.1 The Mon-Jasnow algorithm

In the following we assume periodic boundary conditions in the y direction. That is, the lattice is rolled into a tube so that the $j_m = 1$ and $j_m = N_y$ rows are next to each other. Below, we will discuss the boundary conditions in the x direction.

In 1984, Mon and Jasnow [4] proposed an algorithm for the purpose of measuring the *line tension* in the Ising model [3]. The line tension is defined as the free energy associated with the boundaries between islands (or domains) of spin up and spin down. Mon and Jasnow [4] proposed the following: Prepare *two* square lattices as described above. In both of them, add a row in the y direction with $i_m = 0$. Along this row, all spins are *fixed*, i.e., they do not change, and set to the value $\sigma_{(0,j)} = +1$. Next, in one of the lattices add a row in the

[3] Notice that there is a local download link for this paper given in the list of references.

y direction at $i_m = N_x + 1$ where the spins are fixed, $\sigma_{(N_x+1,j)} = +1$, whereas in the other lattice, the extra row at $(N_x + 1, j)$ has fixed spins with values $\sigma_{(N_x+1,j)} = -1$ [see Fig. 1 of Ref. [4]]. The Hamiltonian, defined in Eq. (1), for the first lattice we denote H_{++}, whereas the Hamiltonian for the second lattice, we denote H_{+-}.

We may now define the free energy associated with the line tension in the Ising model. If F_{++} denotes the free energy associated with the ++ lattice and F_{+-} the free energy associated with the +− lattice, the surface tension free energy τ is

$$N_y\tau = F_{+-} - F_{++}. \tag{2}$$

Intuitively, this is easy to understand since in the +− lattice there *must* be an interface at zero temperature T forced into existence by the boundary conditions in the x direction. The free energies F_{++} and F_{+-} are related to the partition functions (Z_{++} and Z_{+-}) and hence to the Hamiltonians through the expressions

$$\exp\left[-\frac{F_{++}}{k_BT}\right] = Z_{++} = \sum_{\text{conf.}} \exp\left[-\frac{H_{++}}{k_BT}\right], \tag{3}$$

and

$$\exp\left[-\frac{F_{+-}}{k_BT}\right] = Z_{+-} = \sum_{\text{conf.}} \exp\left[-\frac{H_{+-}}{k_BT}\right]. \tag{4}$$

The sums in these two latter equations run over all possible spin configurations (denoted conf.). In the following, we use units so that the Boltzmann constant is $k_B = 1$.

Combining Eq. (2) with Eqs. (3) and (4) gives

$$\tau = -\frac{T}{N_y} \ln \frac{Z_{+-}}{Z_{++}}. \tag{5}$$

The ratio between the two partition functions may be written in the form (which is the main observation made by Mon and Jasnow [4])

$$\frac{Z_{+-}}{Z_{++}} = \frac{\sum_{\text{conf.}} \exp\left[-\dfrac{H_{+-} - H_{++}}{T}\right] \exp\left[\dfrac{-H_{++}}{T}\right]}{Z_{++}} = \left\langle \exp\left[-\frac{H_{+-} - H_{++}}{T}\right] \right\rangle_{++}. \tag{6}$$

This is, the ratio Z_{+-}/Z_{++} equals the average of the quantity $\exp[-(H_{+-} - H_{++})/T]$ in the system governed by the H_{++} Hamiltonian.

The quantity $\langle \exp[-(H_{+-} - H_{++})/T] \rangle_{++}$ we sample numerically using the Metropolis Monte Carlo algorithm [5]. That is, we use the Boltzmann weight $\exp[-H_{++}/T]$ for the probability distribution.

2.2.2 The extended Mon-Jasnow algorithm

So far the Mon-Jasnow algorithm was used for calculating τ. In the following, and for the same purpose, we will consider an extension of this algorithm. We call it the *extended Mon-Jasnow algorithm*. The original Mon and Jasnow algorithm [4] uses two fixed boundary layers at $i_m = 0$ and $i_m = N_x + 1$. These two fixed boundary conditions will disturb the calculation

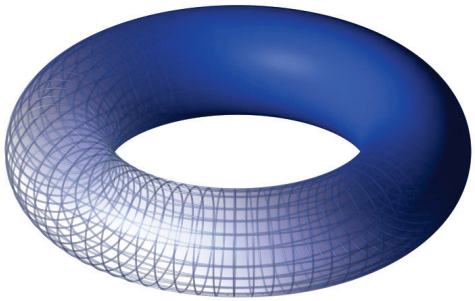

Figure 1: A torus

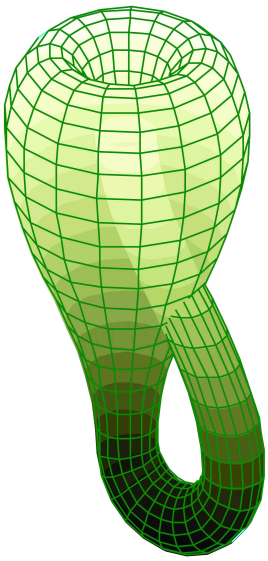

Figure 2: A Klein bottle

for small lattice sizes and getting rid of them would be an improvement. This is the aim of the extended Mon-Jasnow algorithm which can be described in the following way. Use two lattices as in the Mon-Jasnow algorithm. In one of the lattices, use *periodic boundary conditions* also in the x direction. This means that the $i_m = 1$ row is neighbor to the $i_m = N_x$ row in the x direction. Hence, the lattice forms a torus, see Fig. 1. We call the Hamiltonian, Eq. (1), for this system H_t.

The second lattice, we implement on a *Klein bottle*, the structure shown in Fig. 2. This curious structure has only one side. If we cut out a ribbon in the horizontal direction, the ribbon will form an annulus (ring). However, if we cut out a ribbon in the vertical direction, it will form a Möbius strip as shown Fig. 3. The Hamiltonian, Eq. (1), for the Klein bottle we denote H_k.

At temperature $T = 0$, there will be an interface in the Klein bottle system but not in the torus system. Therefore, we may define the free energy associated with the line tension

$$N_y\tau = F_k - F_t, \tag{7}$$

where the subscripts k and t refer to the Klein bottle system and the torus system, respectively.

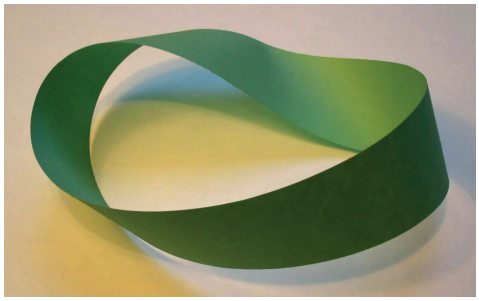

Figure 3: The Möbius strip

By following the step-by-step arguments leading up to Eqs. (5) and (6), we find

$$\tau = -\frac{T}{N_y} \ln \left\langle \exp\left[-\frac{H_k - H_t}{T} \right] \right\rangle_t \tag{8}$$

where the average $\langle \cdots \rangle_t$ is calculated through Metropolis Monte Carlo using the torus system.

It may sound very difficult to implement the Klein bottle boundary conditions. Fortunately, this is not the case. Just connect the node at $j_m = j$ on the $i_m = 1$ row with the node at $j_m = N_y + 1 - j$ on the $i_m = N_x$ row through a *reversed sign* in the coupling constant in the Hamiltonian. Hence, we have $H_k = \ldots - \sigma_{(1,2)}\sigma_{(2,2)} + \sigma_{(1,2)}\sigma_{(N_x,N_y+1-2)} - \ldots$. This is all.

2.3 Close to the critical point

The Ising model on the square lattice has a critical point at a temperature $T_c = 2/\ln(1+\sqrt{2}) \approx 2.2691\ldots$. Below this temperature, the line tension free energy is different from zero, whereas above this temperature, it is zero. If we introduce the reduced temperature

$$t = \frac{T_c - T}{T_c}, \tag{9}$$

the line tension free energy may given the form

$$\tau = \tau_0 t^{\mu} \Sigma\left(N_y^{1/\nu} t \right), \tag{10}$$

for temperatures T below T_c. According to Onsager's famous exact solution of the Ising model on the square lattice [3] the parameters that appear in Eq. (10) have the values $\mu = 1$, $\nu = 1$ and $\tau_0 \approx 3.99\ldots$. Furthermore, the function $\Sigma(z)$ that is present in Eq. (10) is a *scaling function* that approaches 1 as $z \to \infty$ and $\Sigma(z) \sim z^{-\mu}$ when $z \to 0^+$.

2.4 Exam questions

a) Implement the original Mon-Jasnow algorithm and reproduce the results presented in Figs. 3 and 4 of Ref. [4]. If you are able to reproduce these figures, your basic implementation is probably correct and you should be well positioned to start the implementation of the extended Mon-Jasnow algorithm.

From now on and in the rest of this exam, the extended Mon-Jasnow algorithm will be assumed if nothing else is said to indicate otherwise. Below you are asked to use this new algorithm to produce results that are equivalents to those presented in Figs. 3–5 of Ref. [4] and obtained on the basis of the original Mon-Jasnow algorithm.

b) Implement the extended Mon-Jasnow algorithm and describe briefly how you have done it.

c) Plot the line tension τ as a function of temperature T and verify that there is a phase transition at $T = T_c$. Do this for different values of $N \equiv N_y$ (and assume that $N_y = N_x$ so that you change the linear size in both the x and y direction simultaneously). You should see that the transition becoming sharper by increasing value of N .

d) Assume that you are at the critical point $T = T_c$ ($t = 0$) and present τ as a function of N (recall $N \equiv N_y$) in a log-log plot. You should get a straight line with the slope $-\mu/\nu = -1$ (why?). Show this numerically.

e) For a number of different values of t, plot τ/t^μ as a function of $1/(N^{\mu/\nu}t^\mu)$ where you vary N. You should find that all the data fall on a single curve (the master curve) that crosses the y axis at the value $\tau_0 = 3.99\ldots$. Show this numerically and, in particular, give an estimate of the value for τ_0 that you obtain.

Should you prefer, you may alternatively (or in addition) present these data as a τ/t^μ vs. $N^{\mu/\nu}t^\mu$ plot, as is done if Fig. 5 of Ref. [4]. From this plot you should also be able to extract a value for τ_0.

f) Compare the results for (i) τ *vs.* T and (ii) τ *vs.* N [or if you prefer $N\tau$ *vs.* N] obtained on the basis of the original and the extended Mon-Jasnow algorithm. Do you find any differences, if any, between these results obtained by the two algorithms? How do you interpret your findings.

For your information it is mentioned that during grading, subproblems 2(c)–(e) will be given the highest and about equal weights; less weight will be given to subproblems 2(a) and 2(f); and the least weight will be given to 2(b).

References

[1] Assignment 02 can be found at `http://web.phys.ntnu.no/~ingves/Teaching/TFY4235/Assignments/TFY4235_Assignment_02.pdf`

[2] For instance, see `https://en.wikipedia.org/wiki/Square_lattice_Ising_model` and references therein.

[3] L. Onsager, *Crystal statistics. I. A two-dimensional model with an order-disorder transition*, Phys. Rev. **65**, 117 (1944).

[4] K.K. Mon and D. Jasnow, *Direct calculation of interfacial tension for lattice models by the Monte Carlo method*, Phys. Rev. A **30**, 670 (1984). [Download a local copy of the paper from here]

[5] See, for instance, pp. 523 of the course slides `http://web.phys.ntnu.no/~ingves/Teaching/TFY4235/Download/TFY4235_Slides_2020.pdf`